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June 20, 1995

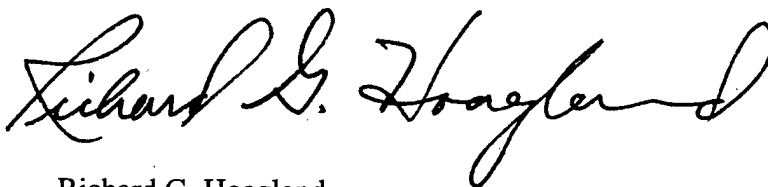
Dr. George R. Yoder
Office of Naval Research
CD 1131
Materials Division, Engineering Sciences
800 N. Quincy St.
Arlington, VA 22217-5000

Ref: Grant N00014-93-1-0022 "Deformation and Fracture Mechanisms in Thin
Films and Beryllium Intermetallics

Dear Dr. Yoder:

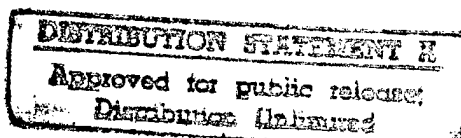
To our dismay we have discovered that the final report for the above-referenced grant had not been submitted and is overdue. Consequently, we have enclosed three copies of the final report for this grant. We apologize for the delay.

Sincerely,



Richard G. Hoagland
Professor

cc: J. P. Hirth, Mechanical and Materials Enggr
C. Zuiches, Office of Grant
and Research Development





DEPARTMENT OF THE NAVY
OFFICE OF NAVAL RESEARCH
SEATTLE REGIONAL OFFICE
1107 NE 45TH STREET, SUITE 350
SEATTLE WA 98105-4631

IN REPLY REFER TO:

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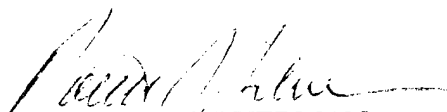
From: Director, Office of Naval Research, Seattle Regional Office, 1107 NE 45th St., Suite 350,
Seattle, WA 98105

To: Defense Technical Center, Attn: P. Mawby, 8725 John J. Kingman Rd., Suite 0944,
Ft. Belvoir, VA 22060-6218

Subj: RETURNED GRANTEE/CONTRACTOR TECHNICAL REPORTS

1. This confirms our conversations of 27 Feb 97 and 11 Jul 97. Enclosed are a number of technical reports which were returned to our agency for lack of clear distribution availability statement. This confirms that all reports are unclassified and are "APPROVED FOR PUBLIC RELEASE" with no restrictions.

2. Please contact me if you require additional information. My e-mail is silverr@onr.navy.mil and my phone is (206) 625-3196.


ROBERT J. SILVERMAN

Final Report

on

**DEFORMATION AND FRACTURE MECHANISMS IN
THIN FILMS AND BERYLLIUM INTERMETALLICS**

Conducted under

Grant N00014 - 93 - 1 - 0022

by

John P. Hirth

Richard G. Hoagland

1995

**Washington State University
Pullman, WA 99164**

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Final Report on

**DEFORMATION AND FRACTURE MECHANISMS IN THIN
FILMS AND BERYLLIUM INTERMETALLICS**

Overview

The overall goal of this program was to investigate the mechanical properties of several Be intermetallics for the purpose of evaluating their suitability for high temperature structural applications. This work was begun May, 1989 and was completed in 1992 with Battelle Pacific Northwest Laboratories as the prime contractor and Washington State University as a subcontractor. At WSU the work was directed by Profs. John Hirth and Richard Hoagland. Subsequent work supported by this grant enabled the completion of the Ph. D. research of two students, Brad Benson and Sanjay Sondhi.

This program enabled the completion of research on the fracture toughness of thin films and the deformation behavior of Be_{12}X compounds. The grant enabled the extension of previous thin film work to include tests of thin brittle films on elastic-plastic substrates in order to measure the fracture toughness of the film and the film-substrate interface. The atomistic modelling had been focused on a study of the atomic arrangement in the core of several different types of dislocations in Be_{12}X . This work was extended to examine the energetics of the transformation of the bct Be_{12}X phase to the rhombohedral Be_{17}X_2 phase by the repeated faulting. There is the potential that this deformation operation could produce a structure with enhanced plasticity.

Fracture Toughness Measurements of Thin Films

A test method for measuring the toughness of attached thin films and the film-substrate interface was developed. The method involved deformation of the substrate under controlled displacement conditions using a test specimen that contains a thin panel of substrate coated with the film. Models of the test specimen allowed the determination of the crack driving forces as a function of the applied displacements and the crack length. The specimen and test is designed such that J decreases as the crack length increases. Thus the test method allows multiple measurements of film cracking, film decohesion, and film crack density saturation on a single specimen.

For Cr films ranging in thickness from 0.2 to 0.9 μm , evaporatively deposited on Al and Cu substrates, the experiments indicate that the toughness of the Cr film varies approximately as the square root of thickness and were in the range of 2.5 to 4.5 $\text{MPa}\sqrt{\text{m}}$. Also Cr films decohered from Cu substrates after film cracking, while they remained attached to Al substrates. The fracture energy of the Cr-Cu interface was found to be about 13 J/m^2 . The effects of substrate plasticity and stable decohesion cracking on the fracture toughness measurements was also examined.

Atomic Simulation of Dislocations in Be_{12}X Compounds

Earlier work in this part of the program involved the development of the relevant atomic potentials using the embedded atom method (EAM). These potentials were subsequently used to model various dislocations and stacking faults in the Be_{12}X bct structure by means of molecular dynamics calculations. One observation from this work concerned the transformation of the crystal structure from bct to base centered orthorhombic and to rhombohedral by a periodic operation of certain slip systems.

TEM observations of Be_{12}Nb that had undergone high temperature deformation had shown that $a/2\langle 100 \rangle$ and $a/2\langle 011 \rangle$ partials are present in very high densities and account for most of the plasticity. Associated with these two partials are stacking faults on the (001) and (011) planes. In our models we find that these faults have a very low energy. In addition, periodic faulting is possible on first the (001) and then (011) planes and this leads to localized phase transformation from the bct to a rhombohedral structure and thence to a base centered orthorhombic structure. The transformation from the bct Be_{12}X phase to the Be_{17}X_2 phase requires diffusion of Be atoms in addition to periodic faulting, thus suggesting the grain boundaries as preferential sites for the nucleation of the transformation. We suggest that alloying additions that favor the rhombohedral Be_{17}X_2 structure would also favor this periodic faulting mechanism, and thus enhance ductility.

Theses Completed

1. Bradley A. Benson, "A method for Fracture Toughness Measurements in Thin Films and Coatings" Ph. D. Thesis, Washington State University, 1993.

2. Sanjay K. Sondhi, "Atomic Scale Modeling of Dislocations in Be_{12}X Compounds", Ph. D. Thesis, Washington State University, 1994.